

# On the physical significance of geometrothermodynamic metrics

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## Abstract

In geometrothermodynamics (GTD), to study the geometric properties of the equilibrium space three thermodynamic metrics have been proposed that are obtained by using the condition of Legendre invariance, and can be computed explicitly once a thermodynamic potential is specified as fundamental equation. We use the remaining diffeomorphism invariance in the phase and equilibrium spaces to show that the components of the GTD-metrics can be interpreted as the second moment of the fluctuation of a new thermodynamic potential. This result establishes a direct connection between GTD and fluctuation theory. In this way, the diffeomorphism invariance of GTD allows us to introduce new thermodynamic coordinates and new thermodynamic potentials which are not related by means of a Legendre transformation to the fundamental thermodynamic potentials.

**Keywords:** Legendre transformations, thermodynamics, geometrothermodynamics, thermodynamic potentials

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## I. INTRODUCTION

Classical equilibrium thermodynamics is based upon a set of empirical observations that became the laws of thermodynamics. This empirical background is probably the cause of the tremendous success of thermodynamics in all possible configurations that can be considered as thermodynamic systems. Although usually a thermodynamic system is specified through its equations of state, an alternative method consists in specifying the fundamental equation from which all the equations of state can be derived [1]. In turn, a fundamental equation is determined by means of a thermodynamic potential  $\Phi$  which is usually understood as a function of the extensive variables  $E^a$ ,  $a = 1, \dots, n$ , where  $n$  is the number of thermodynamic degrees of freedom of the system. Furthermore, it is well known that from a given thermodynamic potential  $\Phi$ , it is possible to obtain a set of new potentials  $\tilde{\Phi}$  by means of Legendre transformations. An important result of classical thermodynamics is that the properties of a system do not depend on the choice of potential. From a theoretical point of view this implies that classical thermodynamics is invariant with respect to Legendre transformations, i.e., it preserves Legendre invariance.

On the other hand, the utilization of differential geometry in classical thermodynamics has shown to be of special importance as an alternative representation and as an additional tool to investigate stability and criticality properties of thermodynamic systems [2–4]. The main idea consists in representing all possible equilibrium states of a system as points of an abstract space that is called equilibrium space. Furthermore, the main goal is to find a relationship between the geometric properties of the equilibrium space and the thermodynamic properties of the system. In this regard, the approach based upon the introduction of specific metrics into the equilibrium space is known as thermodynamic geometry. In particular, one can use the second derivatives of a thermodynamic potential to construct a Hessian matrix which determines a Hessian metric, if its determinant is non-zero. In this way, the equilibrium space becomes a Riemannian manifold with well-defined connection and curvature. One then tries to associate connection and geodesics with quasi-static processes, curvature with thermodynamic interaction and curvature singularities with phase transitions. The interesting issue about using Hessian metrics in the equilibrium space is that they have a very interesting physical significance. In fact, if we consider small fluctuations of the thermodynamic potential, which should be an extremal at each equilibrium point, the second moment

of the fluctuation turns out to be directly related to the components of the corresponding Hessian metric. This is, of course, a very important result of thermodynamic geometry.

A different approach is represented by the formalism of geometrothermodynamics (GTD) whose main feature is that it takes into account the Legendre invariance of classical thermodynamics, a property which is not considered in thermodynamic geometry. To this end, GTD uses the thermodynamic phase space as an auxiliary manifold. However, the GTD-metrics are not Hessian and, therefore, their physical interpretation is not clear. The main goal of the present work, is to show that in GTD it is possible to use the freedom in choosing the coordinates of the phase and equilibrium spaces in order to introduce a new thermodynamic potential and new thermodynamic coordinates such that the metric of the equilibrium space becomes Hessian. This proves that the components of the GTD-metrics can be also interpreted as the second moment of fluctuation of a thermodynamic potential.

This work is organized as follows. In Sec. II, we present a brief review of the formalisms of thermodynamic geometry and GTD, including the general form of the metrics that are used in both formalisms. In Sec. III, we use the diffeomorphism invariance that is left in the phase and equilibrium spaces to obtain the conditions for the GTD-metrics to become Hessian. First, we consider diffeomorphisms that act on the phase space, and introduce the concept of deformed contactomorphisms in order to integrate the differential equations that determine the diffeomorphism. We show that there exists a particular diffeomorphism that transforms the partially and totally Legendre invariant metric of GTD into a Hessian metric at the level of the equilibrium space. The Hessian potential turns out to be a new coordinate introduced by the particular diffeomorphism of the phase space. We then consider the GTD-metrics that are invariant with respect to total Legendre transformations only. We show in Sec. III B that in this case it is necessary to consider the diffeomorphism invariance of the equilibrium space in order to introduce new coordinates that transform the GTD-metrics into Hessian metrics. It turns out that the existence of the Hessian potential in this case depends on the dimension  $n$  of the equilibrium space. If  $n = 2$ , there always exists a Hessian potential, but for  $n \geq 3$  a Hessian potential exists only if the Riemann curvature of the equilibrium space satisfies certain algebraic conditions related to the Pontryagin characteristic class of the manifold. It is then necessary to consider each particular thermodynamic system separately in order to establish the existence of a Hessian potential. In Sec. IV, we propose a new classification of thermodynamic potentials according to their thermodynamic and geometric properties. We

classify thermodynamic potentials into fundamental, Legendre and diffeomorphic potentials. Finally, in Sec. V we discuss our results.

## II. HESSIAN METRICS AND GTD-METRICS

Consider an analytic function  $H(E^a)$ ,  $a = 1, 2, \dots, n$ . In an  $n$ -dimensional manifold, it is possible to introduce a Hessian metric as

$$g^H = \frac{\partial^2 H}{\partial E^a \partial E^b} dE^a dE^b, \quad (1)$$

if the condition  $\det(g_{ab}^H) \neq 0$  is satisfied. If we now consider the set  $\{E^a\}$  as the coordinates of a differential manifold  $\mathcal{E}$  and the function  $H(E^a)$  as a thermodynamic fundamental equation, then  $\mathcal{E}$  can be interpreted as an equilibrium manifold with the Hessian metric (1) determining all the geometric properties of  $\mathcal{E}$ . The function  $H(E^a)$  is also known as the Hessian potential. This is exactly the procedure that is followed in thermodynamic geometry to endow the equilibrium space with a metric.

The physical meaning of the components of Hessian metrics justifies its utilization and leads to a large number of physical applications. Indeed, since a set of values  $E^a$  represents a state of equilibrium in  $\mathcal{E}$ , where from a physical point of view fluctuations are always present, let us denote by  $dE^a$  the infinitesimal deviations of the variables  $E^a$  from the equilibrium state. To take into account the fluctuations of  $H(E^a)$  around an equilibrium state, one basically analyzes the behavior of the Taylor expansion [10]

$$H(E^a + dE^a) = H(E^a) + \frac{\partial H}{\partial E^a} dE^a + \frac{1}{2} \frac{\partial^2 H}{\partial E^a \partial E^b} dE^a dE^b + \dots \quad (2)$$

At equilibrium, the thermodynamic potential reaches an extremal value which can be a maximum or a minimum, depending on the type of thermodynamic potential. Then, the first-order derivatives vanish at equilibrium and the second moment of the fluctuation corresponds basically to the components of the Hessian metric. This can be considered as the mathematical definition of a thermodynamic potential in the framework of fluctuation theory; we will use this definition for the analysis of the new thermodynamic potentials that will be introduced below.

From a physical point of view, however, the interpretation of  $H(E^a)$  as a thermodynamic potential requires the consideration of the properties of the underlying thermodynamic sys-

tem. In fact, for analyzing the physical processes which can occur in a particular thermodynamic system it is necessary to consider it as a part of a larger system which includes the reservoir. At equilibrium, the properties of both the system and the reservoir must be considered and if the additivity condition is satisfied, the potential  $H(E^a)$  splits into two pieces, each possibly with different properties. Then, different arguments must be invoked to show that the second term of the Taylor expansion (2) vanishes at equilibrium. In turn, the arguments depend on the particular physical significance of the potential [10]. For instance, if we choose  $H$  as the entropy  $S$ , then, it must be identified as the entropy of the entire Universe. Moreover, since it reaches a maximum at equilibrium, i.e.,  $\partial S/\partial E^a = 0$ , the second fluctuation moment given in Eq.(2) corresponds basically to the Hessian matrix of the entropy which is known as the Ruppeiner metric [4], and is also interpreted as the stability matrix in fluctuation theory. This important result provides Ruppeiner metric with a clear physical significance, and permits to find the connection with information geometry. Furthermore, if we choose  $H$  as the internal energy  $U$ , a similar argumentation can be used to show that the second term in the Taylor expansion (2) vanishes, and the second moment of the fluctuation  $\frac{\partial^2 U}{\partial E^a \partial E^b}$  determines the components of the Weinhold metric [3], which is related to the Ruppeiner metric by means of a conformal factor. The above description shows the important physical significance of Hessian metrics in thermodynamic geometry.

In GTD, the procedure for introducing Riemannian metrics into the equilibrium space is different. GTD aims to incorporate into a geometric description all the mathematical and physical properties of classical thermodynamics. Therefore, it is necessary to introduce additional structures that make it possible to understand the laws of thermodynamics from a geometric point of view. In the following description, we will use the Legendre invariance property of thermodynamics in order to derive the metrics that are used in GTD to describe physical systems.

In classical thermodynamics, to describe an arbitrary system with  $n$  degrees of freedom, it is necessary to consider  $n$  extensive variables  $E^a$ ,  $n$  intensive variables  $I^a$ , and one thermodynamic potential  $\Phi$ . For a particular system, the corresponding fundamental equation must be specified, which is usually represented by a function that relates the potential with the extensive variables, i.e.,  $\Phi = \Phi(E^a)$ . For the sake of generality, we will demand that  $\Phi(E^a) \in C^\infty$  is an analytical function. The first law of thermodynamics implies then that

(summation over repeated indices)

$$d\Phi = I_a dE^a, \quad I_a = \frac{\partial \Phi}{\partial E^a}. \quad (3)$$

In this way, the intensive variables become explicitly functions of the extensive variables, i.e.,  $I_a = I_a(E^b)$ .

A Legendre transformation is usually represented as a change of potential that includes its first-order derivatives. Consider, for instance, the simple case of a function of only one variable  $\Phi = \Phi(E^1)$ . A Legendre transformation of  $\Phi$  implies the introduction of a new potential  $\tilde{\Phi}$  by means of

$$\Phi \rightarrow \tilde{\Phi} = \Phi - \frac{\partial \Phi}{\partial E^1} E^1. \quad (4)$$

Then, from the first law of thermodynamics we obtain  $d\tilde{\Phi} = -E^1 dI_1$ , implying that

$$\tilde{\Phi} = \tilde{\Phi}(I_1), \quad \text{and} \quad E^1 = -\frac{\partial \tilde{\Phi}}{\partial I_1}. \quad (5)$$

This means that a Legendre transformation affects the functional dependence of the potential and interchanges the role of extensive and intensive variables.

Our goal is to represent Legendre transformations in a pure differential geometric fashion, for instance, as a coordinate transformations. Clearly, the Legendre transformation (4) cannot be interpreted as a change of coordinates because it includes the derivatives of one of the coordinates. It is therefore necessary to introduce an auxiliary space in which all the coordinates are independent. Let us consider the  $(2n+1)$ -dimensional space  $\mathcal{T}$  with coordinates  $Z^A = \{\Phi, E^a, I_a\}$ , where  $A = 0, 1, \dots, 2n$ . Then, the coordinate transformation [5]

$$\{Z^A\} \longrightarrow \{\tilde{Z}^A\} = \{\tilde{\Phi}, \tilde{E}^a, \tilde{I}^a\}, \quad (6)$$

$$\Phi = \tilde{\Phi} - \tilde{E}^k \tilde{I}_k, \quad E^i = -\tilde{I}^i, \quad E^j = \tilde{E}^j, \quad I^i = \tilde{E}^i, \quad I^j = \tilde{I}^j, \quad (7)$$

where  $i \cup j$  is any disjoint decomposition of the set of indices  $\{1, \dots, n\}$ ,  $k, l = 1, \dots, i$ . For  $i = \emptyset$ , we obtain the identity transformation, and for  $i = \{1, \dots, n\}$  a total Legendre transformation, i.e.,

$$\Phi = \tilde{\Phi} - \tilde{E}^a \tilde{I}_a, \quad E^a = -\tilde{I}^a, \quad I^a = \tilde{E}^a. \quad (8)$$

Here we use the notation  $I^a = \delta^{ab} I_b$  with  $\delta_{ab} = \text{diag}(1, \dots, 1)$ . It is then easy to see that if we introduce the dependence  $\Phi = \Phi(E^a)$ , the above coordinate transformation reduces to the

Legendre transformation which includes derivatives of  $\Phi$ . From now on we refer to Eq.(7) as Legendre transformations.

Let us now suppose that  $\mathcal{T}$  is a smooth manifold. Then, by virtue of Darboux's theorem [6], the space  $\mathcal{T}$  with coordinates  $Z^A = \{\Phi, E^a, I_a\}$  can be endowed with a unique (up to a conformal function) differential 1-form  $\Theta = d\Phi - I_a dE^a$  which satisfies the condition  $\Theta \wedge (d\Theta)^n \neq 0$ , and is called contact 1-form. The pair  $(\mathcal{T}, \Theta)$  is known as contact manifold. The interesting point about the canonical contact 1-form is that it is invariant with respect to Legendre transformations, i.e., the new 1-form  $\tilde{\Theta}$ , which is obtained from  $\Theta$  by applying a Legendre transformation (7), can be written as  $\tilde{\Theta} = d\tilde{\Phi} - \tilde{I}_a d\tilde{E}^a$ , implying that the functional dependence of  $\Theta$  remains unchanged. This means that in general a contact manifold is Legendre invariant.

We now introduce a Riemannian metric structure  $G$  into the contact manifold. The triad  $(\mathcal{T}, \Theta, G)$  forms an odd-dimensional Riemannian contact manifold which is the basis for the construction of GTD. Indeed, if we demand that the metric  $G$  be Legendre invariant, i.e., the functional dependence of  $G = G_{AB} dZ^A dZ^B$  should remain invariant under the action of Legendre transformations. The triad  $(\mathcal{T}, \Theta, G)$  constitutes the thermodynamic phase space of GTD [7]. This completes the construction of a Legendre invariant formalism at the level of the phase space which, as we have shown, is an auxiliary manifold we introduced in order for Legendre transformations to be considered as coordinate transformations. The physical space where the thermodynamic systems can be investigated is represented by the equilibrium space  $\mathcal{E}$  which is defined as a submanifold of  $\mathcal{T}$  by means of the embedding smooth map  $\varphi : \mathcal{E} \rightarrow \mathcal{T}$  such that the pullback  $\varphi^*$  satisfies the condition  $\varphi^*(\Theta) = 0$ . Furthermore, if we choose the set  $\{E^a\}$  as the coordinates of the submanifold  $\mathcal{E}$ , then the embedding map reads  $\varphi : \{E^a\} \mapsto \{\Phi(E^a), E^a, I^a(E^a)\}$ , and the condition  $\varphi^*(\Theta) = 0$  implies the first law of thermodynamics (3). Notice that the specification of the map  $\varphi$  implies that the fundamental equation must be given explicitly. In addition, the embedding map  $\varphi$  induces a canonical metric  $g$  on  $\mathcal{E}$  by means of  $g = \varphi^*(G)$ . One of the aims of GTD is to describe the physical properties of a thermodynamic system by using the geometric properties of the corresponding Riemannian equilibrium manifold  $(\mathcal{E}, g)$ .

The above construction of the GTD equilibrium manifold shows that it is completely determined once the metric  $G$  and the fundamental equation  $\Phi(E^a)$  are given. It is therefore necessary to find the explicit form of  $G$  which is invariant under Legendre transformations.



In GTD, we impose an additional physical condition on  $G$ . In the equilibrium manifold, the metric  $g$  is expected to represent the properties of the system; in particular, we want to identify the curvature of  $\mathcal{E}$  as a measure of thermodynamic interaction. This means that  $\mathcal{E}$  must be flat for a system without thermodynamic interaction, i.e., for the ideal gas. Clearly, because of the relation  $g = \varphi^*(G)$ , this demand implies a condition on the form of  $G$ . To carry out this procedure, the problem appears that Legendre transformations are discrete and therefore not all of them can be generated from infinitesimal generators. Moreover, if we limit ourselves to infinitesimal Legendre transformations, the corresponding metric  $G^{inf}$  for the phase space does not lead to a flat metric  $g^{inf} = \varphi^*(G^{inf})$  for the ideal gas [8, 9]. Consequently, it is necessary to apply the general form of the transformation (7) to an arbitrary metric  $G = G_{AB}dZ^AdZ^B$  and demand the functional dependence invariance. The resulting set of algebraic equations [7] can be solved for the metric components  $G_{AB}$  and then the flatness condition for the corresponding metric  $g_{ab}$  can be imposed. As a result, we obtain two different classes of solutions

$$G^{III} = (d\Phi - I_a dE^a)^2 + (\xi_{ab} E^a I^b)(\chi_{cd} dE^c dI^d), \quad (9)$$

which are invariant under total Legendre transformations and a third class (summation over all repeated indices)

$$G^{III} = (d\Phi - I_a dE^a)^2 + (E_a I_a)^{2k+1} dE^a dI^a, \quad k \in \mathbb{Z}, \quad (10)$$

which is invariant under partial Legendre transformations. Here  $\xi_{ab}$  and  $\chi_{ab}$  are diagonal constant  $(n \times n)$ -matrices. If we choose  $\chi_{ab} = \delta_{ab} = \text{diag}(1, \dots, 1)$ , the resulting metric  $G^I$  can be used to investigate systems with at least one first-order phase transition. Alternatively, for  $\chi_{ab} = \eta_{ab} = \text{diag}(-1, \dots, 1)$ , we obtain a metric  $G^{II}$  that correctly describes systems with second-order phase transitions.

To consider the three classes of Legendre invariant metrics in a compact form, we introduce the notation

$$G = \Theta^2 + h_{ab} dE^a dI^b, \quad (11)$$

where the components  $h_{ab}$  are in general functions of  $E^a$  and  $I^a$ . Then, the general form of the metric for the equilibrium manifold can be written as

$$g = \varphi^*(G) = h_{ab} \delta^{bc} \frac{\partial^2 \Phi}{\partial E^c \partial E^d} dE^a dE^d, \quad (12)$$

which is not a Hessian metric.

In contrast to the above construction of GTD, in the alternative approach of thermodynamic geometry, the equilibrium manifold is equipped with a Hessian metric

$$g^H = \frac{\partial^2 \Phi}{\partial E^a \partial E^b} dE^a dE^b, \quad (13)$$

which is not invariant with respect to Legendre transformations. Nevertheless, the components of a Hessian metric have a very clear physical interpretation in fluctuation theory, as described above. The metrics used in GTD (12) are not Hessian due to the presence of the conformal factor determined by the components of  $h_{ab}$ , which on  $\mathcal{E}$  are in general functions of the potential  $\Phi$  and its derivatives.

### III. DIFFEOMORPHISM INVARIANCE

The GTD-metrics of the phase and equilibrium manifolds were obtained under the condition that they preserve Legendre invariance. Their functional dependence is fixed, but we can still perform coordinate transformations without affecting their geometric properties. For instance, in the equilibrium manifold we can apply a diffeomorphism  $\chi : \mathcal{E} \rightarrow \mathcal{E}$ , or in coordinates  $\chi : \{E^a\} \mapsto \{E^{\bar{a}}\}$ , which preserves the properties of  $\mathcal{E}$ . In this work, we will focus on only diffeomorphism which are equivalent to coordinate transformations.

It is clear that in general it is not possible to transform an arbitrary metric like (12) into a Hessian metric by using only the diffeomorphism  $\chi$ . However, the phase manifold offers more possibilities because it is also invariant with respect to coordinate transformations of the form  $\chi_\tau : \{Z^A\} \mapsto \{Z^{\bar{A}}\}$ . For concreteness, let us consider  $\{Z^{\bar{A}}\} = \{F, X^a, Y^a\}$ , where in general  $F = F(\Phi, E^b, I^b)$ ,  $X^a = X^a(\Phi, E^b, I^b)$ , and  $Y^a = Y^a(\Phi, E^b, I^b)$ . In turn, the diffeomorphism  $\chi_\tau$  induces a diffeomorphism  $\chi_\mathcal{E}$  on  $\mathcal{E}$ , according to the diagram represented in Fig. 1.

$$\begin{array}{ccc} (\mathcal{T}, Z^A) & \xrightarrow{\chi_\tau} & (\mathcal{T}, Z^{\bar{A}}) \\ \varphi_E \uparrow & & \uparrow \varphi_X \\ (\mathcal{E}, E^a) & \xrightarrow{\chi_\mathcal{E}} & (\mathcal{E}, X^a) \end{array}$$

Fig. 1: Diagram of maps relating the phase and equilibrium manifolds.

Our goal is to apply a general diffeomorphism  $\chi_{\mathcal{T}}$  on  $\mathcal{T}$  such that the resulting metric can be written as

$$\chi_{\mathcal{T}}(G) = \bar{G} = \chi_{\mathcal{T}}[(d\Phi - I_a dE^a)^2 + h_{ab} dE^a dI^b] = \bar{G}_1 + \delta_{ab} dX^a dY^b, \quad (14)$$

where the first component  $\bar{G}_1$  satisfies the condition

$$\bar{\varphi}_x^*(\bar{G}_1) = 0. \quad (15)$$

The reason for demanding this particular form of the metric is as follows. First, let us note that, according to Darboux's theorem, the introduction of the coordinates  $\{Z^{\bar{A}}\} = \{F, X^a, Y^a\}$  implies that there exists a canonical contact form  $\Theta^F = f(dF - Y_a dX^a)$ , where  $f$  is a non-zero function  $f : \mathcal{T} \rightarrow \mathbb{R}$ . Then, we can introduce a smooth map  $\bar{\varphi}_x : \mathcal{E} \rightarrow \mathcal{T}$  such that  $\bar{\varphi}_x^*(\Theta^F) = 0$ , implying that

$$dF = Y_a dX^a = \frac{\partial F}{\partial X^a} dX^a \quad (16)$$

on  $\mathcal{E}$ . Consequently, taking into account the condition  $\bar{\varphi}_x^*(\bar{G}_1) = 0$ , it can be seen that the metric induced by the pullback  $\bar{\varphi}_x^*$  on  $\mathcal{E}$  reads

$$\bar{g} = \bar{\varphi}_x^*(\bar{G}) = \bar{\varphi}_x^*(\delta_{ab} dX^a dY^b) = \frac{\partial^2 F}{\partial X^a \partial X^b} dX^a dX^b, \quad (17)$$

i.e., it is a Hessian metric. This would imply that in principle we can associate the components of the GTD-metrics with the second fluctuation moment of  $F$ , if it can be considered as a thermodynamic potential.

We notice that the conditions (14) and (15) are sufficient for the induced metric  $\bar{g}$  to become Hessian. In the following sections, we will analyze this condition in the particular case of the GTD-metrics.

### A. Deformed contactomorphisms

To perform the above procedure for determining the explicitly form of the diffeomorphism  $\chi_{\mathcal{T}}$ , it is necessary to carry out lengthy computations involving partial differential equations. The method rapidly becomes cumbersome and difficult to be carried out. To facilitate the analysis of the problem, we make some simplifying assumptions. When applying the

diffeomorphism  $\chi_{\mathcal{T}}$  on the general form of the metric  $G$  given in Eq.(11), let us assume that the following conditions are satisfied

$$\chi_{\mathcal{T}}(d\Phi - I_a dE^a) = f(dF - Y_a dX^a) , \quad (18)$$

$$\chi_{\mathcal{T}}(h_{ab} dE^a dI^b) = \delta_{ab} dX^a dX^b . \quad (19)$$

These assumptions satisfy identically the general conditions (14) and (15). If the above assumptions are satisfied, the map  $\chi_{\mathcal{T}}$  becomes a contactomorphism, i.e., a diffeomorphism that preserves the contact structure. The first assumption (18) leads to a system of  $2n + 1$  partial differential equations

$$\frac{\partial F}{\partial \Phi} = \frac{1}{f} + Y_a \frac{\partial X^a}{\partial \Phi} , \quad \frac{\partial F}{\partial E^a} = -\frac{I_a}{f} + Y_b \frac{\partial X^b}{\partial E^a} , \quad \frac{\partial F}{\partial I^a} = Y_b \frac{\partial X^b}{\partial I^a} , \quad (20)$$

whose integrability conditions can be expressed as

$$\{X^a, Y_a\}_{\Phi E^b} = 0 , \quad \{X^a, Y_a\}_{\Phi I^b} = 0 , \quad \{X^a, Y_a\}_{E^b I^c} = \frac{\delta_{bc}}{f} , \quad (21)$$

where

$$\{Z^{\bar{A}}, Z^{\bar{B}}\}_{Z^A Z^B} = \frac{\partial Z^{\bar{A}}}{\partial Z^A} \frac{\partial Z^{\bar{B}}}{\partial Z^B} - \frac{\partial Z^{\bar{A}}}{\partial Z^B} \frac{\partial Z^{\bar{B}}}{\partial Z^A} . \quad (22)$$

The above integrability conditions resemble the conditions for a transformation of generalized coordinates and momenta to be a canonical transformation in classical mechanics. This is due to the fact that any section of  $\mathcal{T}$  with fixed  $\Phi$  (or  $F$ ) corresponds to a symplectic manifold with a symplectic structure similar to that of the phase space in classical mechanics.

We now consider the assumption (19). It is straightforward to write down explicitly the corresponding system of partial differential equations in which we can insert the integrability conditions (21). As a result, we obtain

$$(X^a, Y_a)_{\Phi \Phi} = (X^a, Y_a)_{\Phi E^b} = (X^a, Y_a)_{\Phi I^b} = (X^a, Y_a)_{E^b E^c} = 0, \quad (X^a, Y_a)_{E^b I^c} = \frac{1}{2} h_{bc} - \frac{\delta_{bc}}{f}, \quad (23)$$

where the round parenthesis represent the operator

$$(Z^{\bar{A}}, Z^{\bar{B}})_{Z^A Z^B} = \frac{\partial Z^{\bar{A}}}{\partial Z^A} \frac{\partial Z^{\bar{B}}}{\partial Z^B} . \quad (24)$$

We thus have derived in Eqs.(20) and (23) the explicit differential equations for the contactomorphism conditions (18) and (19) to be satisfied.

If we now insert the different values of the components  $h_{ab}$  into the above differential equations, lengthy calculations show that they are not satisfied in general for any of the GTD-metrics, the integrability conditions being one of the main problems. Nevertheless, a detailed study of the analytic form of the integrability conditions show that they are satisfied if we allow the contact form to be subject to a “deformation” of the form

$$\bar{\Theta} \rightarrow f_0 dF - f_a Y_a dX^a, \quad (25)$$

where the non-vanishing functions  $f_0$  and  $f_a$  can depend on all coordinates  $F$ ,  $X^a$  and  $Y^a$ . In other words, if we relax the contactomorphism condition (18), and instead assume that

$$\chi_{\mathcal{T}}(d\Phi - I_a dE^a) = f_0 dF - f_a Y_a dX^a, \quad (26)$$

the integrability conditions are satisfied. It then follows that condition (14) should be “deformed” into

$$\bar{G} = (f_0 dF - f_a Y_a dX^a)^2 + \delta_{ab} dX^a dY^b, \quad (27)$$

for the integrability conditions to be satisfied. Consequently, we demand that the line element for the phase space  $\mathcal{T}$  in the new coordinates  $Z^{\bar{A}}$  has exactly this form in accordance with the requirements of the integrability conditions in terms of the deformed contactomorphism.

Let us consider the corresponding equilibrium space  $\mathcal{E}$  by means of the embedding map  $\bar{\varphi}_x : \mathcal{E} \rightarrow \mathcal{T}$  which is defined by the condition  $\bar{\varphi}_x^*(dF - Y_a dX^a) = 0$ . Then, the thermodynamic metric  $\bar{g} = \bar{\varphi}_x^*(\bar{G})$  induced in  $\mathcal{E}$  can be expressed as

$$\bar{g} = (f_0 - f_a)(f_0 - f_b) \frac{\partial F}{\partial X^a} \frac{\partial F}{\partial X^b} dX^a dX^b + \frac{\partial^2 F}{\partial X^a \partial X^b} dX^a dX^b. \quad (28)$$

We see that this metric is not Hessian because it contains also first-order derivatives of the new coordinate  $F(X^a)$ . Moreover, it depends on  $n + 1$  arbitrary functions  $f_0$  and  $f_a$ . Nevertheless, if we now demand that  $F(X^a)$  reaches an extremal value at equilibrium, i.e.,  $\partial F / \partial X^a = 0$  with  $\frac{\partial^2 F}{\partial X^a \partial X^b} \neq 0$  at each point of the equilibrium manifold, then the metric  $\bar{g}$  reduces to

$$\bar{g} = \frac{\partial^2 F}{\partial X^a \partial X^b} dX^a dX^b, \quad (29)$$

i.e., it becomes Hessian. As discussed in Sec. II, to interpret the function  $F(X^a)$  as a thermodynamic potential from a physical point of view further requirements must be imposed,

namely, that  $F$  corresponds to the potential of the entire universe, whereas  $X^a$  corresponds to the thermodynamic subsystem described by the metric (29).

This result shows that for the metric of the equilibrium manifold to become Hessian, it is necessary not only that the new coordinate  $F(X^a)$  be introduced as an element of a diffeomorphism, but also that it can be interpreted as thermodynamic potential, according to the mathematical definition given in Sec. II. Indeed, consider the infinitesimal fluctuations  $dX^a$  of the potential  $F(X^a)$  around an equilibrium state  $X^a$ . Then, taking into account that at equilibrium  $F(X^a)$  is extremal, we obtain up to the second approximation order the Taylor expansion

$$F(X^a + dX^a) = F(X^a) + \frac{1}{2} \frac{\partial^2 F}{\partial X^a \partial X^b} dX^a dX^b . \quad (30)$$

We conclude that the components of the GTD-metrics in the equilibrium space can be interpreted as the second fluctuation moment of the new thermodynamic potential  $F$ , which is generated by a diffeomorphism of the phase space, satisfying the condition (26) of a deformed contactomorphism,  $\chi_\tau(d\Phi - I_a dE^a) = f_0 dF - f_a Y_a dX^a$ , and acting on the second part of the general GTD-metric as

$$\chi_\tau(h_{ab} dE^a dI^b) = \delta_{ab} dX^a dX^b . \quad (31)$$

Consider now the last condition. One can see that  $\bar{h} = \delta_{ab} dX^a dX^b$  represents a well-defined line element in a  $2n$ -dimensional manifold  $\mathcal{C}$ , with coordinates  $\{E^a, I^a\}$ , which is known as the control manifold. Since in this particular case the metric  $\delta_{ab}$  is constant, the control manifold is flat. This implies that the curvature of the metric  $h = \chi_\tau^{-1}(\bar{h}) = h_{ab} dE^a dI^b$  must vanish as well. A direct computation of the GTD-metrics shows that this condition is satisfied only by the metric  $G^{III}$ . Indeed, in this case we have that only the diagonal components of  $h_{ab}$  are non-vanishing and are given as  $h_{aa} = (E_a I_a)^{2k+1}$ ; consequently, the corresponding manifold is flat.

Condition (31) implies that in the case of the metric  $G^{III}$  the diffeomorphism is determined by the relations

$$F = \Phi, \quad X^a = \frac{(E^a)^{2k+2}}{2k+2}, \quad Y^a = \frac{(I^a)^{2k+2}}{2k+2}, \quad (32)$$

whereas the deformed contactomorphism is given by

$$f_0 = 1, \quad f_a = (2k+2)^{-\frac{2k+1}{k+1}} (X^a Y^a)^{-\frac{2k+1}{2k+2}} . \quad (33)$$

We thus see that in the case of the metric  $G^{III}$ , the new thermodynamic potential  $F(X^a)$  coincides with the original potential  $\Phi$ ; however, its explicit functional dependence on the coordinates is different.

It is easy to see that in the case of the GTD-metrics  $G^I$  and  $G^{II}$ , the second part of the metric,  $h_{ab}dE^a dE^b$ , does not correspond to a flat control manifold. It is therefore necessary to apply a different approach.

## B. Hessian manifolds

According to the results presented in the last subsection, the GTD-metrics  $G^I$  and  $G^{II}$ , which are invariant with respect to total Legendre transformations, cannot induce a Hessian metric in  $\mathcal{E}$ , independently of coordinate system chosen in the phase manifold  $\mathcal{T}$ . We therefore consider the general form of the induced metric in terms of the extensive variables  $E^a$ . From Eq.(9), we obtain

$$g^{I/II} = \varphi^*(G^{I/II}) = \left( \xi_a^b E^a \frac{\partial \Phi}{\partial E^b} \right) \left( \chi_a^c \frac{\partial^2 \Phi}{\partial E^b \partial E^c} dE^a dE^b \right), \quad (34)$$

with

$$\xi_a^b = \xi_{ac} \delta^{cb}, \quad \chi_a^b = \chi_{ac} \delta^{cb}. \quad (35)$$

The question we need to ask now is whether there exists a coordinate transformation  $E^a \rightarrow X^a = X^a(E^b)$  such that the above metric becomes Hessian, i.e., it transforms into

$$g^{I/II} = \frac{\partial^2 F^{I/II}}{\partial X^a \partial X^b} dX^a dX^b, \quad (36)$$

where  $F^{I/II} = F^{I/II}(X^a)$  is the Hessian potential. To answer this question, it is necessary to invoke the theory of affine connections and dual connections on the equilibrium space  $\mathcal{E}$ . It turns out that a simple answer is not possible because it depends on the dimension of  $\mathcal{E}$ . In fact, the following theorems must be used to investigate this question [17].

**Theorem 1.** All analytic 2-dimensional metrics are Hessian.

If the system under consideration is characterized by two thermodynamic degrees of freedom ( $n = 2$ ), and the fundamental equation  $\Phi = \Phi(E^1, E^2)$  is an analytic function, the condition of the theorem is satisfied and, consequently, there exists a new potential  $F^{I/II} = F^{I/II}(X^1, X^2)$ , with  $X^1 = X^1(E^1, E^2)$  and  $X^2 = X^2(E^1, E^2)$  in which the metric becomes Hessian (36). Many important thermodynamic systems are included in this class;

for instance, the ideal gas and the van der Waals gas [16] with a fixed number of particles, the Reissner-Nordström and the Kerr black hole [19], all the perfect fluids that are used in relativistic cosmology [20], etc.

**Theorem 2.** In 3 dimensions, all possible Riemann curvature tensors occur as the curvature tensor of a Hessian metric.

In the case of a system with three thermodynamic degrees of freedom ( $n = 3$ ), this theorem shows that the curvature of the corresponding thermodynamic metric is equivalent to the curvature of a Hessian metric. Nevertheless, it does not imply the existence of the underlying Hessian potential. Consequently, in such a case it is necessary to consider the explicit form of the Hessian curvature and use the integrability conditions to determine the Hessian potential by using, for instance, the Cartan formalism [18].

**Theorem 3.** In 4 and higher dimensions, for a given metric to be Hessian it is necessary that its Riemann curvature tensor satisfies the conditions

$$\alpha(R_{ija}{}^b R_{klb}{}^a) = 0 , \quad (37)$$

$$\alpha(R_{iajb} R_k{}^b{}_{cd} R_l{}^{dac} - 2R_{iajb} R_{kc}{}^a{}_d R_l{}^{dbc}) = 0 , \quad (38)$$

where the operator  $\alpha$  denotes antisymmetrization of the indices  $i, j, k, l$ . The above conditions are equivalent to demanding that the Pontryagin forms, associated with the Pontryagin characteristic class, vanish on a Hessian manifold [17]. This is due to the fact that Hessian manifolds possess a very particular set of affine connections which annihilates the Pontryagin characteristic class.

If the number of thermodynamic degrees of freedom of the system is  $n \geq 4$ , the fulfillment of the above conditions can be considered as an indication of the existence of a Hessian potential.

The above theorems can be used to find the Hessian potential  $F^{I/II}$  for any given thermodynamic metric  $g^{I/II}$ . Only in the case of  $n = 2$ , it is possible to prove the existence of the Hessian potential in general. In the remaining cases, additional conditions must be satisfied which can be corroborated only if the fundamental equation  $\Phi = \Phi(E^a)$  is given explicitly. This means that in principle there could be systems with  $n \geq 3$  for which no Hessian potential exists. This should be tested for each system separately.

If, in addition, the Hessian potential is characterized by reaching an extremum at equilibrium, it can be interpreted also as a thermodynamic potential and, consequently, the



components of the GTD-metric for the equilibrium space can be interpreted as the second fluctuation moment of the Hessian potential.

#### IV. CLASSIFICATION OF THERMODYNAMIC POTENTIALS

For investigating the physical significance of the GTD-metrics, it was necessary to introduce new thermodynamic potentials by using coordinate transformations. To distinguish the different types of potentials that can be used in thermodynamics and in the geometric representations of thermodynamics, we propose to classify them as fundamental, Legendre and diffeomorphic potentials, according to the following definitions.

*Fundamental potentials:* These are potentials which are given as fundamental equations, i.e., as functions that depend on extensive variables only  $\Phi = \Phi(E^a)$ . This means that there exist only two fundamental potentials which can be identified as the entropy  $S$  and the internal energy  $U$ . In classical thermodynamics, the use of the fundamental potentials lead to the well-known entropy and energy representations, respectively [1]. In thermodynamic geometry, the fundamental potentials entropy and internal energy are used as Hessian potentials to define theuppeiner and Weinhold metrics, respectively.

*Legendre potentials:* These are potentials  $\tilde{\Phi}$  that can be obtained from the fundamental potentials  $\Phi = \Phi(E^a)$  by means of Legendre transformations defined as

$$\Phi = \tilde{\Phi} - \tilde{E}^k \tilde{I}_k, \quad E^i = -\tilde{I}^i, \quad E^j = \tilde{E}^j, \quad I^i = \tilde{E}^i, \quad I^j = \tilde{I}^j, \quad (39)$$

where  $i \cup j$  is any disjoint decomposition of the set of indices  $\{1, \dots, n\}$ ,  $k, l = 1, \dots, i$ . Legendre potentials  $\tilde{\Phi}$  are characterized by depending on at least one intensive variable. The limiting case in which it depends on only intensive variables,  $\tilde{\Phi} = \tilde{\Phi}(I^a)$  corresponds to a total Legendre transformation for which  $i = \{1, 2, \dots, n\}$ . In general, for a system of  $n$  thermodynamic degrees of freedom one can introduce up to  $n^2 - 1$  different Legendre potentials. In GTD, the main idea is that one can use any fundamental or Legendre potential to describe the geometric properties of the equilibrium manifold.

*Diffeomorphic potentials:* These are potentials that can be obtained by applying coordinate transformations on the GTD-metrics under the condition that the resulting metric for the equilibrium manifold is Hessian. There are two ways to generate diffeomorphic potentials by means of coordinate transformations either at level of the phase space, as explained in

Sec. III A, or at the level of the equilibrium space, as explained in Sec. III B. Diffeomorphic potentials are Hessian and simultaneously thermodynamic. They are important because the second moment of their fluctuation determines the components of the GTD-metrics. The diffeomorphic potentials appear as a consequence of the diffeomorphism invariance of the phase and equilibrium manifolds as defined in GTD. The number of possible diffeomorphic potentials is quite large. In principle, as shown in Sec. III A, a Legendre potential can become a diffeomorphic potential after the application of a coordinate transformation on the phase manifold.

## V. CONCLUSIONS

In this work, we analyze the physical significance of the GTD-metrics from the point of view of fluctuation theory. We have seen that imposing Legendre invariance and the condition that the equilibrium manifold of a non-interacting thermodynamic system is flat, we end up with only three different metrics for the phase manifold, namely,  $G^I$  and  $G^{II}$ , which are invariant with respect to total Legendre transformations, and  $G^{III}$ , which is invariant with respect to arbitrary Legendre transformations.

We have shown that in the case of the metric  $G^{III}$ , it is always possible to perform a coordinate transformation at the level of the phase manifold of GTD such that the metric induced in the equilibrium manifold becomes Hessian in terms of a new thermodynamic potential and new coordinates. Our analysis shows that the components of the GTD-metrics at the level of the equilibrium manifold can be interpreted as the second fluctuation moment of the new thermodynamic potential with respect to the new coordinates. We found the explicit form of the new thermodynamic potential and the new coordinates for an arbitrary metric  $G^{III}$ .

In the case of the metrics  $G^I$  and  $G^{II}$ , it is not possible to find the explicit form of the new thermodynamic potential in general. Instead, for each thermodynamic system with a given fundamental equation the calculations must be carried out separately at the level of the equilibrium manifold. We use several theorems about the properties of Hessian manifolds to show that for systems with two degrees of freedom, it is always possible to find a Hessian potential. In the case of a higher number of degrees of freedom, the Riemann curvature of the equilibrium manifold must satisfy certain conditions in order for the Hessian potential

to exist. If, in addition, the Hessian potential possesses an extremum at equilibrium, it becomes the new thermodynamic potential which determines the physical significance of the GTD-metrics components.

The diffeomorphism invariance of the metrics used in GTD allows us to introduce a new type of thermodynamic potential which depends on coordinates not necessarily associated with the usual thermodynamic variables. Moreover, this result can be used to classify thermodynamic potentials into fundamental, Legendre and diffeomorphic potentials. Fundamental and Legendre potentials are used in classical thermodynamics which is invariant with respect to the change of potentials within this class. Diffeomorphic potentials are different because they are obtained by applying arbitrary coordinate transformations on the phase or equilibrium manifolds. The important point is that the components of the GTD-metrics correspond to the second fluctuation moment of diffeomorphic potentials.

Whereas fundamental and Legendre potentials have a clear physical significance, diffeomorphic potentials have been introduced by using the mathematical properties of the phase and equilibrium manifolds. Their physical significance is therefore not yet completely clear. In the case of the metric  $G^{III}$ , however, the diffeomorphic potential is just a fundamental or a Legendre potential written in terms of new coordinates; its physical meaning is therefore closely related to that of the known potentials of classical thermodynamics. In the case of the metrics  $G^I$  and  $G^{II}$ , it is necessary to perform the explicit calculation of the diffeomorphic potential for each particular system in order to investigate its physical meaning.

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